



# STIC Search Report

## Biotech-Chem Library

STIC Database Tracking Number: 10/731108

**TO:** Rei-Tsang Shiao  
**Location:** rem/5A10/5C18  
**Art Unit:** 1626  
**Tuesday, January 31, 2006**

**Case Serial Number:** 10/731108

**From:** Mary Hale  
**Location:** Biotech/Chem Library  
**Rem 1D86**  
**Phone:** 2-2507

**Mary.Hale@uspto.gov**

### Search Notes

Feel free to contact me if you have any questions.

Note -- results are printed on both sides of printout



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Page 1

Shias

10/73/108

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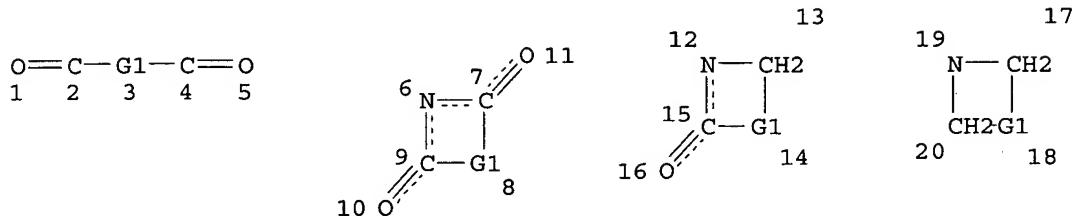
(FILE 'HOME' ENTERED AT 16:10:59 ON 31 JAN 2006)

FILE 'CASREACT' ENTERED AT 16:11:08 ON 31 JAN 2006

L1 STR  
L2 STR L1  
L3 0 S L2  
L4 2 S L2 FUL

=> d 12 que stat

L2 STR



REP G1=(2-4) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

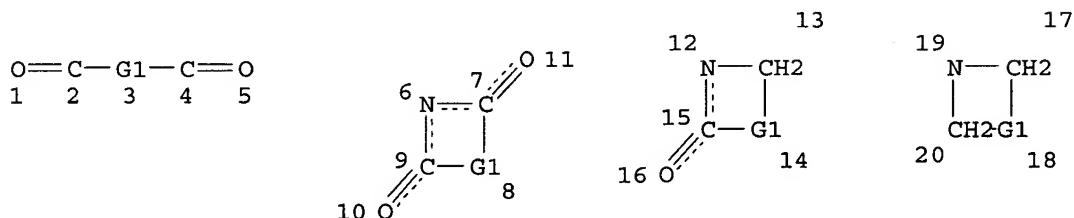
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

=> d 13 que stat

L2 STR



REP G1=(2-4) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L3 0 SEA FILE=CASREACT SSS SAM L2 ( 0 REACTIONS)

100.0% DONE 3276 VERIFIED 0 HIT RXNS

0 DOCS

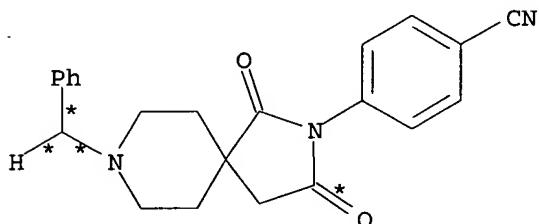
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 62097 TO 68943  
PROJECTED ANSWERS: 0 TO 0

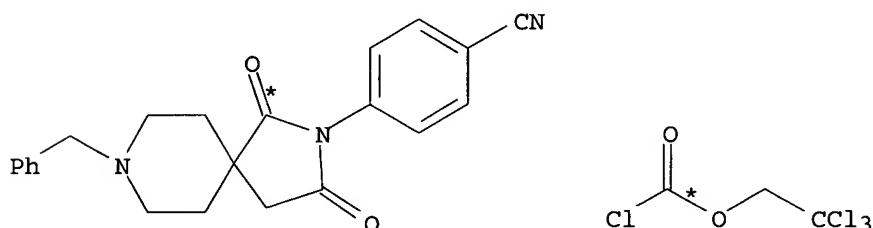
=> d 14 fhit ibib abs

L4 ANSWER 1 OF 2 CASREACT COPYRIGHT 2006 ACS on STN

RX(163) OF 590 COMPOSED OF RX(5), RX(6), RX(7), RX(14)  
RX(163) 2 O + 2 X + AR ==> AS

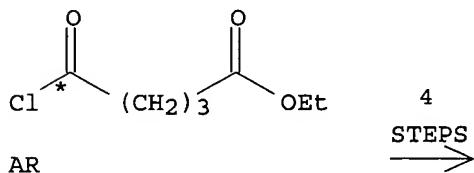


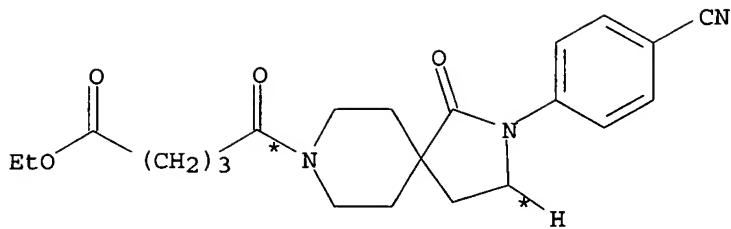
O



O

2 X





AS  
YIELD 92%

RX(5) RCT O 685544-29-0

STAGE(1)

RGT T 16940-66-2 NaBH4  
 SOL 67-56-1 MeOH  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 0 deg C -> room temperature  
 SUBSTAGE(3) room temperature

STAGE(2)

RGT U 64-19-7 AcOH

STAGE(3)

RGT T 16940-66-2 NaBH4  
 SOL 76-05-1 F3CCO2H  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 0 deg C -> room temperature  
 SUBSTAGE(3) room temperature

PRO R 685544-31-4, S 685544-30-3

NTE reaction is extremely vigorous in third stage

RX(6) RCT S 685544-30-3, R 685544-31-4, X 17341-93-4

PRO Y 685544-33-6, Z 685544-32-5

SOL 75-05-8 MeCN, 75-09-2 CH2Cl2

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) overnight, room temperature

NTE 85% overall yield, 8:2 mixture of starting lactams used

RX(7) RCT Z 685544-32-5

RGT AC 631-61-8 NH4OAc

PRO AB 685544-34-7

SOL 109-99-9 THF, 7732-18-5 Water

CON SUBSTAGE(1) room temperature, pH 5

SUBSTAGE(2) room temperature

NTE Cd-Pb couple used

RX(14) RCT AB 685544-34-7, AR 5205-39-0

RGT AT 7087-68-5 EtN(Pr-i)2

PRO AS 685544-38-1

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 0 deg C -> room temperature

SUBSTAGE(3) 4 hours, room temperature

ACCESSION NUMBER: 140:385509 CASREACT

TITLE: Discovery of Novel 2,8-Diazaspiro[4.5]decanes as Orally Active Glycoprotein IIb-IIIa Antagonists  
AUTHOR(S): Mehrotra, Mukund M.; Heath, Julie A.; Smyth, Mark S.; Pandey, Anjali; Rose, Jack W.; Seroogy, Joseph M.; Volkots, Deborah L.; Nannizzi-Alaimo, Lisa; Park, Gary L.; Lambing, Joseph L.; Hollenbach, Stanley J.; Scarborough, Robert M.  
CORPORATE SOURCE: Millennium Pharmaceuticals Inc., South San Francisco, CA, 94080, USA  
SOURCE: Journal of Medicinal Chemistry (2004), 47(8), 2037-2061  
CODEN: JMCMAR; ISSN: 0022-2623  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

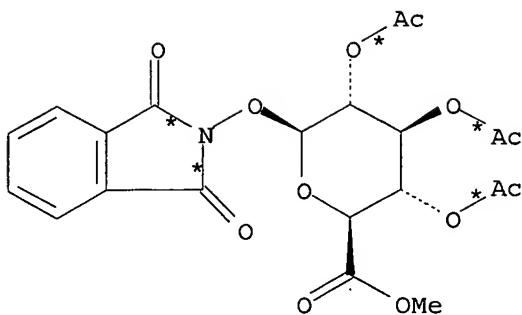
AB In our efforts to develop orally active GPIIb-IIIa antagonists with improved pharmaceutical properties, we have utilized a novel 2,8-diazaspiro[4.5]decane scaffold as a template. We describe here our investigation of a variety of templates including spiropiperidinyl- $\gamma$ -lactams, spiropiperidinylimide, spiropiperidinylureas, and spiropiperidinylhydantoins. With the appropriate acidic and basic pharmacophores in place, each template yielded analogs with potent GPIIb-IIIa inhibitory activity. One of the compds., 59 (CT50787), was also used to demonstrate for the first time the use of a pharmacol. agent which is  $\alpha$ IIb $\beta$ 3 specific to display biol. activity in a lower species such as mouse and to extend bleeding times. Evaluation of the pharmacokinetic properties of selected compds. from each series in rat, dog, and cynomolgus monkey has led to the identification of 22 (CT51464), a double prodrug, with excellent pharmacokinetic properties. It exhibited good pharmacokinetic profile across species (F% = 33 (Cyno), 73 (dog), 22 (rat); t<sub>1/2</sub> $\beta$  = 14.2 h (Cyno), 8.97 h (dog), 1.81 h (rat)). The biol. active form, 23 (CT50728), displayed inhibition of platelet aggregation in platelet rich plasma (PRP) with an IC<sub>50</sub> value of 53 nM in citrate buffer, 110 nM in PPACK anticoagulated PRP, and 4 nM in solid-phase GPIIb-IIIa competition binding assay (ELISA). Both 23 and 22 were stable in human liver microsomes, did not inhibit the P 450 3A4 isoenzyme, and had low protein binding (18.22% for 23) and a desirable log P (0.45 $\pm$ 0.06 for 22, and -0.91 $\pm$ 0.32 for 23). It is predicted that the high oral bioavailability for these compds. in multiple species should translate into lower intra- and intersubject variability in man. The long plasma half-life of the lead is consistent with once or twice daily administration for chronic therapy. Analog 22 (CT51464) thus appears to be a promising oral GPIIb-IIIa inhibitor with significantly improved pharmacokinetic properties over the previously described clin. candidates and may be found useful in the treatment of arterial occlusive disorders.

REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

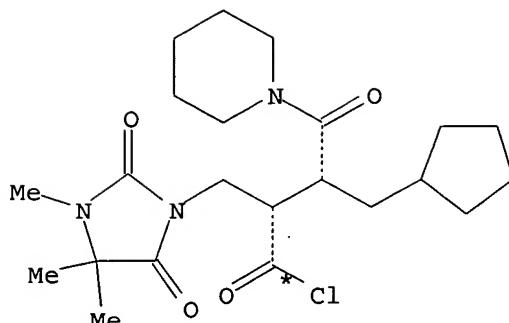
=> d 14 fhit ibib abs 2

L4 ANSWER 2 OF 2 CASREACT COPYRIGHT 2006 ACS on STN

RX(35) OF 82 COMPOSED OF RX(4), RX(6), RX(7), RX(10)  
RX(35) K + R ==> AD

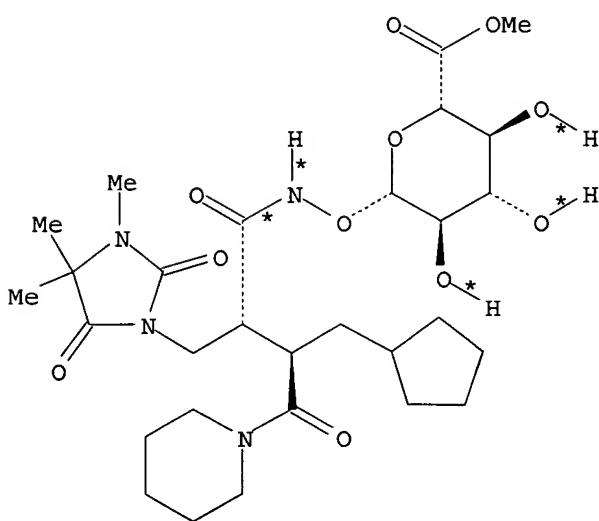


K



R

4  
STEPS  
→



AD  
YIELD 92%

RX (4)      RCT K 319926-19-7  
 RGT P 302-01-2 N2H4  
 PRO O 319926-20-0  
 SOL 67-56-1 MeOH  
 NTE STEREOSELECTIVE

RX (6)      RCT R 319926-22-2, O 319926-20-0  
 RGT W 121-44-8 Et3N  
 PRO V 319926-23-3  
 SOL 75-09-2 CH2Cl2  
 NTE STEREOSELECTIVE

RX(7) RCT V 319926-23-3

STAGE (1)

RGT E 124-41-4 NaOMe  
SOL 67-56-1 MeOH

STAGE (2)

PRO X 319926-24-4  
NTE DUOLITE RESIN (H+FORM) USED IN SECOND STAGE , STEREOSELECTIVE

RX(10) RCT X 319926-24-4

STAGE (1)

RGT AE 25952-53-8 EDAP, AF 2592-95-2 1-Benzotriazolol, AG  
872-50-4 NMEP, Q 174265-77-1 1-Piperidinebutanoic  
acid,  $\beta$ -(cyclopentylmethyl)- $\gamma$ -oxo- $\alpha$ -  
[(3,4,4-trimethyl-2,5-dioxo-1-imidazolidinyl)methyl]-,  
( $\alpha$ R, $\beta$ R)-

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE (2)

RGT E 124-41-4 NaOMe  
SOL 67-56-1 MeOH

STAGE (3)

PRO AD 319926-26-6  
NTE DUOLITE RESIN (H+FORM) USED IN LAST STAGE , STEREOSELECTIVE

ACCESSION NUMBER:

134:116168 CASREACT

TITLE:

The synthesis of the glucuronide adduct of Trocade

AUTHOR(S):

Mitchell, Mark B.; Whitcombe, Ian W. A.

CORPORATE SOURCE:

Chemical Synthesis Department, Roche Discovery Welwyn,  
Welwyn Garden City, AL7 3AY, UK

SOURCE:

Tetrahedron Letters (2000), 41(45), 8829-8834

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The synthetic preparation of the glucuronide adduct of Trocade, a selective inhibitor of the MMP collagenase, is described. This was achieved by preparation of the protected O-glucuronsyl hydroxylamine and subsequent coupling to the available carboxylic acid, followed by deprotection. The synthetic material was identical to authentic isolated metabolite, which confirmed that glucuronidation of Trocade occurs on the oxygen of the hydroxamic acid.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s werpy ?/au  
L5 6 WERPY ?/AU

=> d 1-6 ibib abs

L5 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN

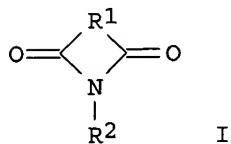
ACCESSION NUMBER: 141:123556 CASREACT

TITLE: Process for producing N-methylsuccinimide from dicarbonyl compounds by cyclization and alkylation and

INVENTOR(S) : hydrogenation to N-methylpyrrolidinone  
Werpy, Todd A.; Frye, John G., Jr.; White,  
James F.; Holladay, Johnathan E.; Zacher, Alan H.  
PATENT ASSIGNEE(S) : Battelle Memorial Institute, USA  
SOURCE: PCT Int. Appl., 31 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004058708	A1	20040715	WO 2003-US40106	20031216
WO 2004058708	B1	20040923		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004176589	A1	20040909	US 2003-731108	20031210
EP 1572644	A1	20050914	EP 2003-814062	20031216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRIORITY APPLN. INFO.:				
US 2002-435469P 20021220				
US 2003-108336 20031210				
US 2003-731108 20031210				
WO 2003-US40106 20031216				

OTHER SOURCE(S) : MARPAT 141:123556  
GI



AB The invention includes methods of processing an initial di-carbonyl compound by conversion to a cyclic compound I (R1 = linear or branched, saturated or unsatd. hydrocarbon or substituted hydrocarbon; R2 = H; linear, cyclic or branched, saturated or unsatd. alkyl; aromatic group). The cyclic compound is reacted with an alkylating agent to form a derivative having an alkylated ring nitrogen. The invention encompasses a method of producing an N-alkyl product. Ammonia content of a solution is adjusted to produce a ratio of ammonia to dicarboxylate compound of from about 1:1 to about 1.5:1. An alkylating agent is added and the initial compound is alkylated and cyclized. The invention includes methods of making N-methylpyrrolidinone (NMP). Aqueous ammonia and succinate is introduced into a vessel and ammonia is adjusted to provide a ratio of ammonia to succinate of less than 2:1. A methylating agent is reacted with succinate at a temperature of from greater

than 100° to about 400° to produce N-methylsuccinimide which is purified and hydrogenated to form NMP.

L5 ANSWER 2 OF 6 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 141:25334 CASREACT  
TITLE: Methods of forming alpha, beta-unsaturated acids and esters  
INVENTOR(S): Lilga, Michael A.; Werpy, Todd A.; Holladay, Johnathan E.  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 9 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004110974	A1	20040610	US 2002-315404	20021209
PRIORITY APPLN. INFO.:			US 2002-315404	20021209

OTHER SOURCE(S): MARPAT 141:25334

AB In the method, a carboxylic acid is mixed with an  $\alpha$ -hydroxy acid or an  $\alpha$ -hydroxy ester and is esterified to form an  $\alpha$ -acyloxy derivative. The  $\alpha$ -acyloxy derivative is transformed into an  $\alpha, \beta$ -unsatd. derivative. The invention addnl. includes a process of forming an acrylate. Lactic acid or a lactic acid ester is reacted with a first portion of acetic acid in the presence of a first catalyst to produce the corresponding 2-acetoxy propionic acid or ester. A non-reacted portion of the acetic acid is recycled. The 2-acetoxypropionic acid or ester is transferred to a second vessel containing a second catalyst, and acetic acid is liberated from the 2-acetoxypropionic acid or ester to produce a corresponding acrylic acid or acrylate ester. The acid or ester is subsequently esterified by reaction with an alc. to form a desired acrylate ester.

L5 ANSWER 3 OF 6 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 138:339970 CASREACT  
TITLE: Hydrogenolysis of 6-carbon sugars and other organic compounds using multimetallic catalysts  
INVENTOR(S): Werpy, Todd A.; Frye, John G., Jr.; Zacher, Alan H.; Miller, Dennis J.  
PATENT ASSIGNEE(S): Battelle Memorial Institute, USA; Michigan State University  
SOURCE: PCT Int. Appl., 40 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003035582	A1	20030501	WO 2002-US33982	20021023
WO 2003035582	B1	20031211		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,  
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,  
 UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,  
 FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,  
 CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 US 2003119952 A1 20030626 US 2001-836 20011023  
 US 6841085 B2 20050111  
 EP 1440046 A1 20040728 EP 2002-784244 20021023  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK  
 PRIORITY APPLN. INFO.: US 2001-836 20011023  
 WO 2002-US33982 20021023  
 AB Methods for hydrogenolysis are described which use a Re-containing  
 multimetallic catalyst for hydrogenolysis of both C-O and C-C bonds.  
 Methods and compns. for reactions of hydrogen over a Re-containing catalyst  
 with compns. containing a 6-carbon sugar, sugar alc., or glycerol are  
 described. It has been surprisingly discovered that reaction with  
 hydrogen over a Re-containing multimetallic catalyst resulted in superior  
 conversion and selectivity to desired products such as propylene glycol.  
 REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 6 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 137:325152 CASREACT  
 TITLE: Hydrogenolysis of 5-carbon sugars, sugar alcohols, and  
 other methods and compositions for reactions involving  
 hydrogen  
 INVENTOR(S): Werpy, Todd A.; Frye, John G., Jr.; Zacher,  
 Alan H.; Miller, Dennis J.  
 PATENT ASSIGNEE(S): Battelle Memorial Institute, USA  
 SOURCE: U.S., 18 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6479713	B1	20021112	US 2001-12890	20011023
US 2003130545	A1	20030710	US 2002-214983	20020806
US 6677385	B2	20040113		
WO 2003035593	A1	20030501	WO 2002-US33983	20021023
WO 2003035593	B1	20031113		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1440048	A1	20040728	EP 2002-786487	20021023
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			

US 2004064003 A1 20040401 US 2003-676497 20030930  
PRIORITY APPLN. INFO.: US 2001-12890 20011023  
US 2002-214983 20020806  
WO 2002-US33983 20021023

AB Methods and compns. for reactions of hydrogen over a Re-containing catalyst with compns. containing a 5-carbon sugar, sugar alc., or lactic acid are described. It has been surprisingly discovered that reaction with hydrogen over a Re-containing multimetallic catalyst resulted in superior conversion and selectivity to desired products such as propylene glycol (PG). A process for the synthesis of PG from lactate or lactic acid is also described.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 6 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 137:5076 CASREACT  
TITLE: Biorefinery concept development based on wheat flour milling  
AUTHOR(S): Elliott, Douglas C.; Orth, Rick J.; Gao, Johnway; Werpy, Todd A.; Eakin, David E.; Schmidt, Andrew J.; Neuenschwander, Gary G.; Flagg, Anthony J.; Murry, Jim; Lahman, Lyle; Lin, C. J.; Mennel, Donald L.; Landucci, Ron  
CORPORATE SOURCE: Pacific Northwest National Laboratory, Richland, WA, 99352, USA  
SOURCE: Preprints of Symposia - American Chemical Society, Division of Fuel Chemistry (2002), 47(1), 361-362  
CODEN: PSADFZ; ISSN: 1521-4648  
PUBLISHER: American Chemical Society, Division of Fuel Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB An overview describing the production of polyols or lactic acid using a wheat millfeed as a source of raw starch. Starch was extract from wheat millfeed using hot water followed by filtration to remove the fibrous material contained in the extract. The fibrous material was found to be useful as an animal feed byproduct. The raw starch was then enzymically liquefied and saccharified to produce dextrose. The dextrose then served as a substrate for fermentation to produce lactic acid or for catalytic hydrogenation to produce sorbitol.

L5 ANSWER 6 OF 6 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 136:340398 CASREACT  
TITLE: Alpha-ester compounds and their thermal decomposition into acrylates and lactones or anhydrides  
INVENTOR(S): Werpy, Todd A.; Lilga, Michael A.  
PATENT ASSIGNEE(S): Battelle Memorial Institute, USA  
SOURCE: PCT Int. Appl., 15 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002032849	A2	20020425	WO 2001-US31570	20011009
WO 2002032849	A3	20020718		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,  
 RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,  
 VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
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 US 6545175 B1 20030408 US 2000-691143 20001019  
 AU 2002013078 A5 20020429 AU 2002-13078 20011009  
 EP 1328502 A2 20030723 EP 2001-981437 20011009  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 CN 1529690 A 20040915 CN 2001-820734 20011009  
 BR 2001014593 A 20050111 BR 2001-14593 20011009  
 PRIORITY APPLN. INFO.: US 2000-691143 20001019  
 WO 2001-US31570 20011009  
 OTHER SOURCE(S): MARPAT 136:340398  
 AB Alpha-ester compds. R3O2CC(R2) [O2CC(R9)(R8)(CR7R6)nC(R4)(R3)CO2R1]C(R10)(R11)(R12) [n = 0, 1; R2-R12 = H, C1-10 alkyl(oxy), C6-10 aryl(oxy), aralkyl; R1 = H, C1-10 alkyl, C6-10 aryl, aralkyl], which decompose at >200° to an acrylate and a lactone or anhydride (no data; where the lactone or anhydride has a b.p. of <170°/1 atmospheric), are prepared. Thus, Me lactate and succinic anhydride were heated to 70° in the presence of sulfuric acid, methanol and chloroform added, and the mixt refluxed to give Me 1-(methoxycarbonyl)ethyl succinate in 98.5% yield.

=> => dis his

(FILE 'HOME' ENTERED AT 16:10:59 ON 31 JAN 2006)

FILE 'CASREACT' ENTERED AT 16:11:08 ON 31 JAN 2006

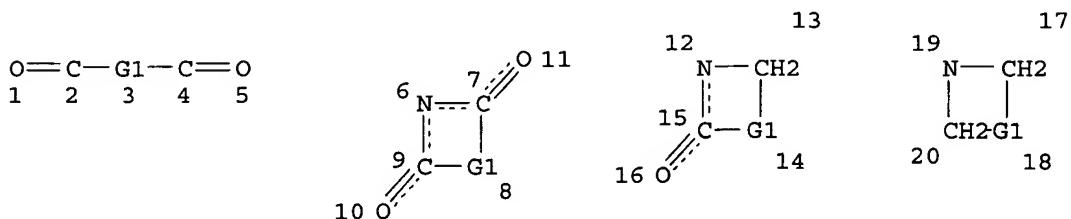
L1 STR  
 L2 STR L1  
 L3 0 S L2  
 L4 2 S L2 FUL  
 L5 6 S WERPY ?/AU

FILE 'CASREACT' ENTERED AT 16:20:25 ON 31 JAN 2006

L6 STR L3  
 L7 50 S L6  
 L8 2816 S L6 FUL  
 L9 STR L2  
 L10 9 SEARCH L9 SUB=L8 FUL  
 L11 7 S L10 NOT L4

=> d 111 que stat

L2 STR



REP G1=(2-4) C

Page 12

NODE ATTRIBUTES:

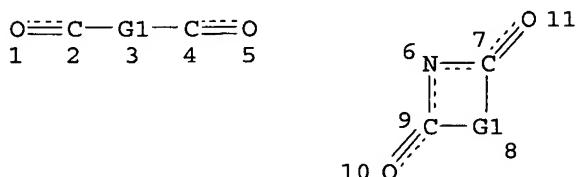
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L4 2 SEA FILE=CASREACT SSS FUL L2 ( 42 REACTIONS)  
L6 STR



REP G1=(2-4) C

NODE ATTRIBUTES:

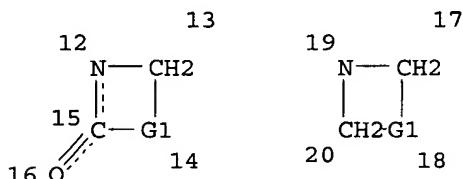
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

L8 2816 SEA FILE=CASREACT SSS FUL L6 ( 52585 REACTIONS)  
L9 STR



REP G1=(2-4) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L10 9 SEA FILE=CASREACT SUB=L8 SSS FUL L9 ( 124 REACTIONS)  
L11 7 SEA FILE=CASREACT ABB=ON PLU=ON L10 NOT L4

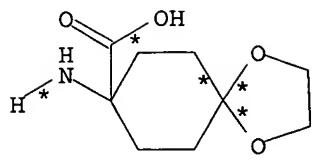
=> d 1-7 fhit ibib abs

L11 ANSWER 1 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

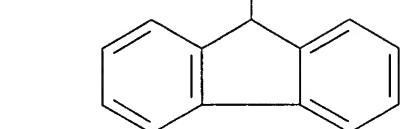
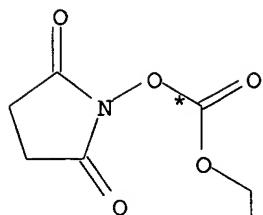
RX(21) OF 22 COMPOSED OF RX(8), RX(9), RX(5)

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

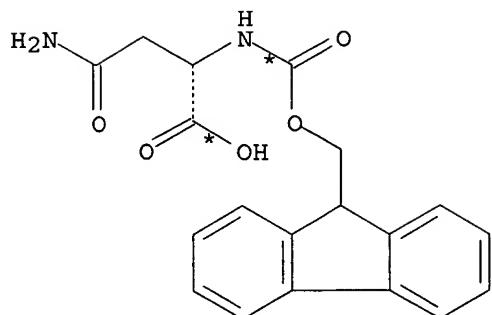
RX(21) AT + AL + AD + C + AE ==> AF



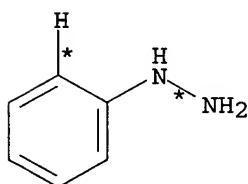
AT



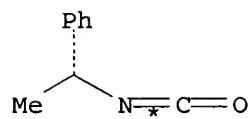
AL



AD

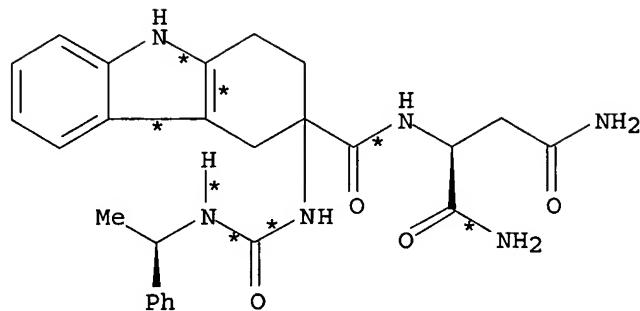


C



AE

3  
STEPS  
→



AF

RX (8) RCT AT 54621-18-0, AL 82911-69-1

STAGE (1)

RGT AP 121-44-8 Et3N, AO 1310-73-2 NaOH  
SOL 7732-18-5 Water, 75-05-8 MeCN  
CON overnight, room temperature, pH 9

STAGE (2)

RGT AR 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, acidify

PRO AU 369403-24-7

RX (9) RCT AU 369403-24-7

RGT AR 7647-01-0 HCl  
PRO B 285996-74-9  
SOL 7732-18-5 Water, 67-64-1 Me2CO  
CON 4 hours, room temperature

RX (5) RCT AD 71989-16-7

STAGE (1)

RGT G 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, hexafluorophosphate(1-),  
3-oxide, H 109-02-4 N-Methylmorpholine  
SOL 68-12-2 DMF

STAGE (2)

RGT I 110-89-4 Piperidine  
SOL 68-12-2 DMF

STAGE (3)

RCT B 285996-74-9  
RGT G 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, hexafluorophosphate(1-),  
3-oxide, H 109-02-4 N-Methylmorpholine  
CAT 1122-58-3 4-DMAP  
SOL 68-12-2 DMF

STAGE (4)

RCT C 100-63-0  
RGT J 64-19-7 AcOH, K 7646-85-7 ZnCl2, L 872-50-4  
NMEP  
CON 20 hours, 70 deg C

STAGE (5)

RGT I 110-89-4 Piperidine  
SOL 68-12-2 DMF

STAGE (6)

RCT AE 33375-06-3  
SOL 107-06-2 ClCH2CH2Cl  
CON 18 hours, room temperature

STAGE (7)

RGT O 76-05-1 F3CCO2H

PRO AF 846567-74-6

NTE reactant bound onto resin

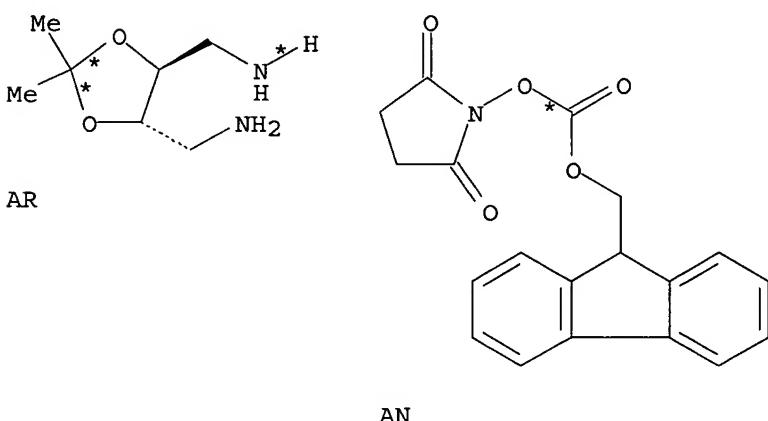
ACCESSION NUMBER: 142:261363 CASREACT  
 TITLE: Solid-phase synthesis of substituted  
 3-amino-3'-carboxytetrahydrocarbazoles  
 AUTHOR(S): Koppitz, Marcus; Reinhardt, Gabriele; van Lingen,  
 Anneke  
 CORPORATE SOURCE: Automated Medicinal Chemistry, Schering AG, Berlin,  
 13342, Germany  
 SOURCE: Tetrahedron Letters (2005), 46(6), 911-914  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

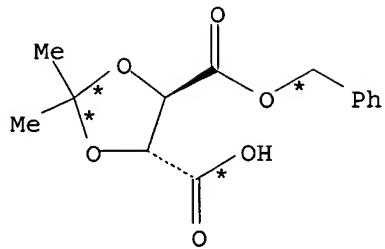
AB Two related solid-phase synthesis routes have been developed allowing the synthesis of 3-amino-3'-carboxy substituted tetrahydrocarbazole derivs. Diversity can be introduced at the amino and carboxy functionalities and at the nitrogen and the aromatic ring of the tetrahydrocarbazole moiety. Both routes rely on Fmoc-protected 1-amino-4-oxocyclohexanecarboxylic acid as central core element. Derivatization of the carboxy function is achieved with amines; derivatization of the amino functionality is possible by reaction with alkyl halides, isocyanates, activated alcs., sulfonic acid chlorides or carboxylic acids. The tetrahydrocarbazole scaffold is generated by Fischer indole cyclization with phenylhydrazine derivs., thereby introducing diversity in the aromatic moiety. N-Alkylation at the indole nitrogen with alkyl halides delivers N-substituted derivs.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

RX(80) OF 248 COMPOSED OF RX(15), RX(17), RX(24)  
 RX(80) AR + AN + AV + BT ==> BZ





AV

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

3

STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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RX(15) RCT AR 119322-88-2, AN 82911-69-1  
RGT AP 121-44-8 Et3N  
PRO AS 675606-43-6  
SOL 109-99-9 THF  
CON 30 minutes, 0 deg C

RX(17) RCT AS 675606-43-6, AV 197457-57-1  
RGT BA 132705-51-2 Phosphorus(1+), bromotri-1-pyrrolidinyl-, (T-4)-, hexafluorophosphate(1-), BB 7087-68-5 EtN(Pr-i)2  
PRO AZ 675606-44-7  
SOL 68-12-2 DMF  
CON 17 hours, room temperature

RX(24) RCT AZ 675606-44-7

STAGE(1)  
RGT BA 132705-51-2 Phosphorus(1+), bromotri-1-pyrrolidinyl-, (T-4)-, hexafluorophosphate(1-), BB 7087-68-5 EtN(Pr-i)2, BV 872-50-4 NMEP  
SOL 75-09-2 CH2Cl2  
CON 4 hours, room temperature

STAGE(2)  
RGT BW 108-24-7 Ac2O, BV 872-50-4 NMEP  
SOL 75-09-2 CH2Cl2  
CON 3 hours, room temperature

STAGE(3)  
RGT BX 110-89-4 Piperidine  
SOL 75-09-2 CH2Cl2, 68-12-2 DMF  
CON 3 hours, room temperature

STAGE (4)

RCT BT 635287-20-6  
RGT BY 2592-95-2 1-Benzotriazolol, BI 25952-53-8 EDAP  
SOL 68-12-2 DMF  
CON 6 hours, room temperature

STAGE (5)

RGT BW 108-24-7 Ac20  
SOL 68-12-2 DMF  
CON 1 hour, room temperature

PRO BZ 758718-14-8D

NTE solid-supported reaction, attachment of spacer (first two stages) repeated up to three times, first stage attachment to TOYOPEARL or AffiGel resin

ACCESSION NUMBER: 141:273853 CASREACT

TITLE: Design and synthesis of novel hydrophilic spacers for the reduction of nonspecific binding proteins on affinity resins

AUTHOR(S): Shiyama, Takaaki; Furuya, Minoru; Yamazaki, Akira; Terada, Tomohiro; Tanaka, Akito

CORPORATE SOURCE: Chemistry Department, Reverse Proteomics Research Institute Co., Ltd, Chiba, 292-0818, Japan

SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(11), 2831-2841

PUBLISHER: CODEN: BMECEP; ISSN: 0968-0896  
Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Tubulin and actin often bind nonspecifically to affinity chromatog. resins, complicating research toward identifying the cellular targets. Reduction of nonspecific binding proteins is important for success in finding such targets. We herein disclose the design, synthesis, and effectiveness in reduction of nonspecific binding proteins, of novel hydrophilic spacers (2-5), which were introduced between matrixes and a ligand. Among them, tartaric acid derivative (5) exhibited the most effective reduction of nonspecific binding proteins, while maintaining binding of the target protein.

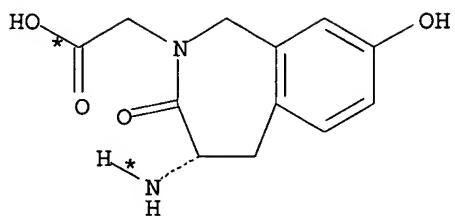
Introduction of 5 on TOYOPEARL reduced tubulin and actin by almost 65% and 90% compared to that without the hydrophilic spacer, resp., with effective binding to the target protein, FKBP12.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

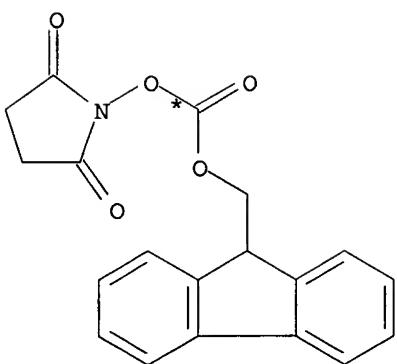
L11 ANSWER 3 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

RX(14) OF 31 COMPOSED OF RX(8), RX(4)

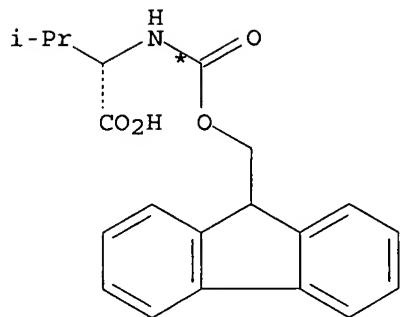
RX(14) AC + AF + A + 4 B + 2 D ==> T



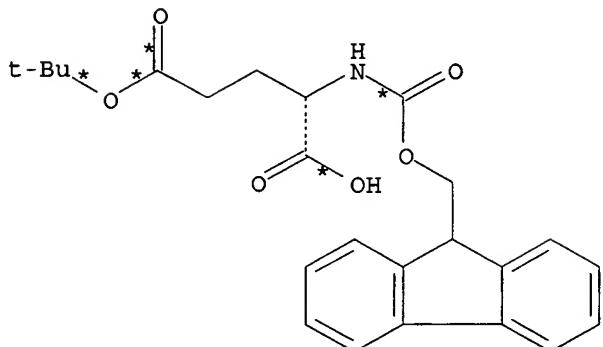
AC



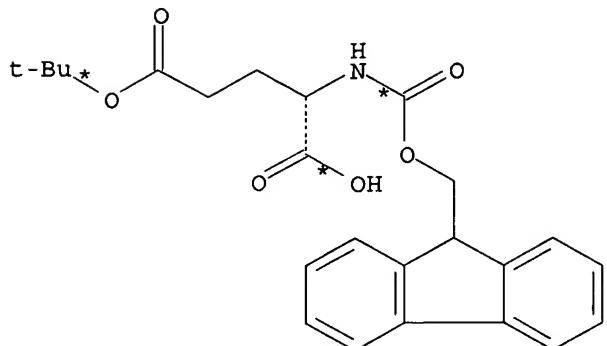
AF



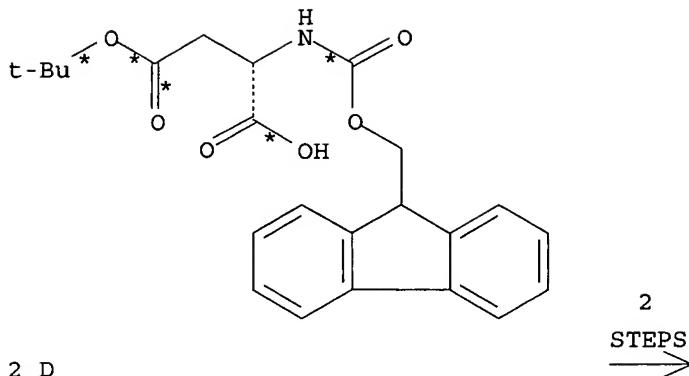
A



B

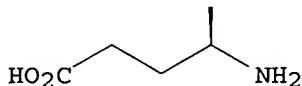


3 B



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PAGE 2-A



T

RX(8) RCT AC 446255-98-7, AF 82911-69-1  
 RGT AG 497-19-8 Na<sub>2</sub>CO<sub>3</sub>  
 PRO S 446255-99-8  
 SOL 7732-18-5 Water, 123-91-1 Dioxane  
 CON overnight, room temperature

RX(4) RCT A 68858-20-8

STAGE(1)  
 SOL 68-12-2 DMF

STAGE(2)  
 RGT F 110-89-4 Piperidine  
 CON 24 minutes, room temperature

STAGE(3)  
 RCT B 71989-18-9  
 RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol  
 SOL 68-12-2 DMF

STAGE(4)  
 RGT F 110-89-4 Piperidine  
 CON 24 minutes, room temperature

STAGE(5)  
 RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol  
 SOL 68-12-2 DMF

STAGE(6)  
 RGT F 110-89-4 Piperidine  
 CON 24 minutes, room temperature

STAGE(7)

RCT S 446255-99-8  
RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol  
SOL 68-12-2 DMF

STAGE(8)

RGT F 110-89-4 Piperidine  
CON 24 minutes, room temperature

STAGE(9)

RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol  
SOL 68-12-2 DMF

STAGE(10)

RGT F 110-89-4 Piperidine  
CON 24 minutes, room temperature

STAGE(11)

RCT D 71989-14-5  
RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol  
SOL 68-12-2 DMF

STAGE(12)

RGT F 110-89-4 Piperidine  
CON 24 minutes, room temperature

STAGE(13)

RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol  
SOL 68-12-2 DMF

STAGE(14)

RGT F 110-89-4 Piperidine  
CON 24 minutes, room temperature

STAGE(15)

RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol  
SOL 68-12-2 DMF

STAGE(16)

RGT F 110-89-4 Piperidine  
CON 24 minutes, room temperature

STAGE(17)

RGT I 6485-79-6 Silane, tris(1-methylethyl)-, J 7732-18-5  
Water, K 76-05-1 F3CCO2H, L 100-66-3 PhOMe

PRO T 446256-02-6

NTE solid-supported reaction, attachment to Wang resin in first  
stage, reactants assumed in seventh, eleventh, thirteenth stages

ACCESSION NUMBER: 140:107390 CASREACT

TITLE: Conformational constraints of tyrosine in protein  
tyrosine kinase substrates: Information about  
preferred bioactive side-chain orientation

AUTHOR(S): Ruzza, Paolo; Calderan, Andrea; Donella-Deana,  
Arianna; Biondi, Barbara; Cesaro, Luca; Osler,  
Alessio; Elardo, Stefano; Guiotto, Andrea; Pinna,  
Lorenzo A.; Borin, Gianfranco

CORPORATE SOURCE: Padova Unit, CNR, Institute of Biomolecular Chemistry,  
Padua, 35131, Italy

SOURCE: Biopolymers (2003), 71(4), 478-488

CODEN: BIPMAA; ISSN: 0006-3525

PUBLISHER: John Wiley & Sons, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The side-chain orientation of a tyrosine residue located in a peptide, which is an excellent substrate of Syk tyrosine kinase, was fixed in the gauche (+) or gauche (-) conformation by using the 7-hydroxy-1,2,3,4-tetrahydro isoquinoline-3-carboxylic (Htc) structure. The tyrosine trans conformation was blocked by using an aminobenzazepine-type (Hba) structure. The proposed side-chain orientations were confirmed by the anal. of the 1H-NMR parameters: chemical shifts, coupling consts., and nuclear Overhauser effects to the tyrosine constraints in the different analogs. This "rotamer scan" of the phosphorylatable residue allowed us to generate optimal substrates in terms of both phosphorylation efficiency and selectivity for Syk tyrosine kinase. In contrast, these conformationally restricted tyrosine analogs were not tolerated by the Src-related tyrosine kinases Lyn and c-Fgr.

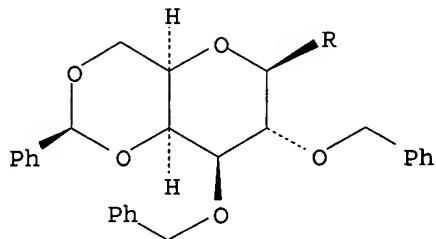
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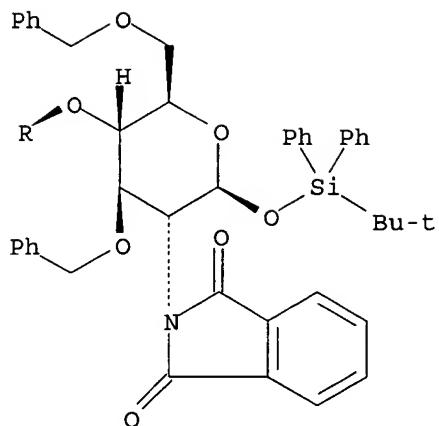
L11 ANSWER 4 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

RX(125) OF 275 COMPOSED OF RX(10), RX(11), RX(12), RX(2), RX(23), RX(24),  
RX(25), RX(16)

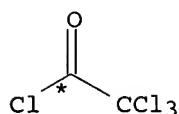
RX(125) AF + AK + BZ + 2 AS + BA + BB + BC + BD + BE + BF  
====> BG

PAGE 1-A

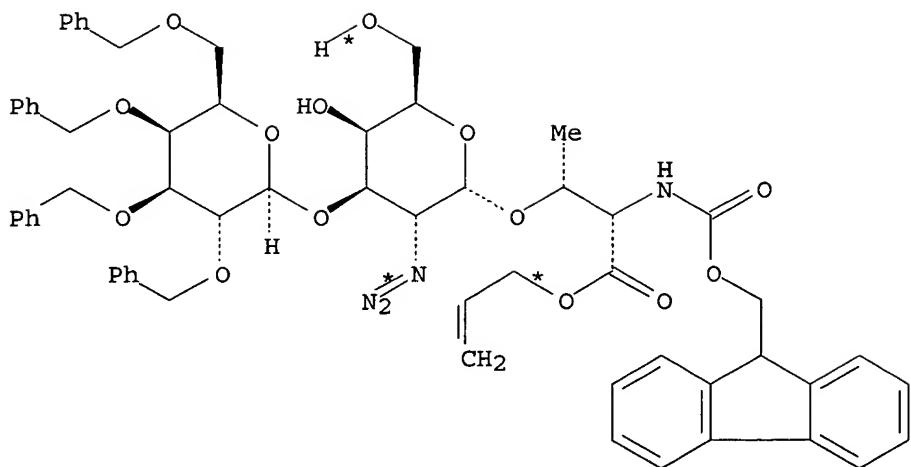




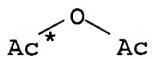
AF



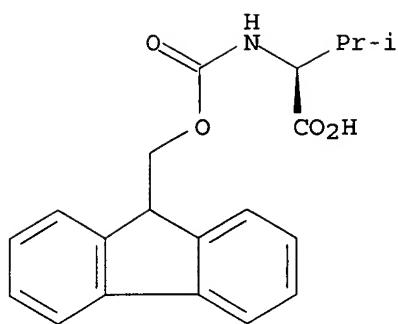
AK



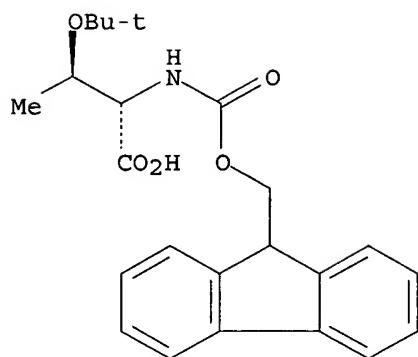
BZ



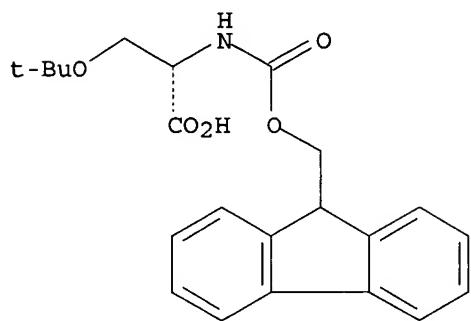
2 AS



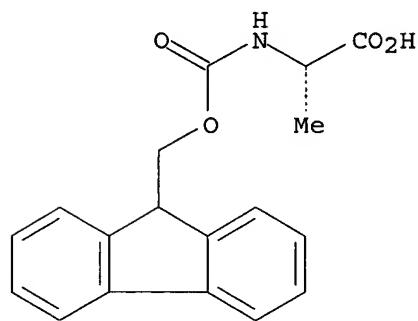
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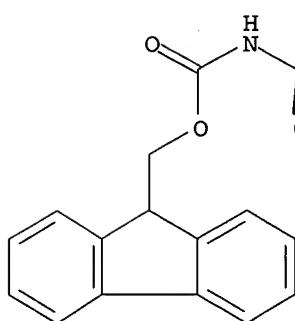
BB



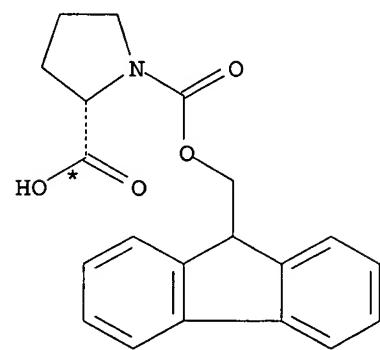
BC



BD



BE

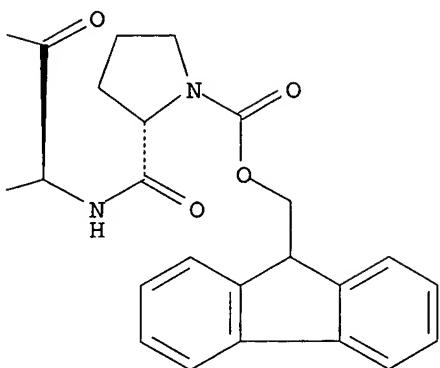


BF

8  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 1-B



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(10) RCT AF 503830-97-5  
RGT AI 107-15-3 H2NCH2CH2NH2  
PRO AH 503830-98-6  
SOL 71-36-3 BuOH  
CON 18 hours, 95 deg C  
NTE alternative prepn. shown

RX(11) RCT AH 503830-98-6, AK 76-02-8  
RGT AM 110-86-1 Pyridine  
PRO AL 503830-99-7  
CON overnight, 0 deg C

RX(12) RCT AL 503830-99-7  
RGT AN 429-41-4 Bu4N.F  
PRO E 620964-97-8  
SOL 109-99-9 THF, 64-19-7 AcOH  
CON overnight, room temperature  
NTE stereoselective

RX(2) RCT E 620964-97-8

STAGE (1)  
RGT G 38078-09-0 DAST [(Et2N).SF3]  
SOL 109-99-9 THF  
CON 30 minutes, 0 deg C

STAGE (2)  
RGT H 67-56-1 MeOH

PRO F 503831-01-4  
NTE stereoselective

RX(23) RCT BZ 503830-92-0

STAGE (1)  
RGT AQ 1291-32-3 ZrCp2Cl<sub>2</sub>, AR 7783-93-9 AgClO<sub>4</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 1 hour, -15 deg C

STAGE (2)  
RCT F 503831-01-4  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 2.5 hours, room temperature

STAGE (3)  
RGT L 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water

PRO CA 503831-03-6

RX (24) RCT CA 503831-03-6

STAGE (1)  
RGT AT 7440-66-6 Zn, AO 64-19-7 AcOH  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 72 hours, room temperature

STAGE (2)  
RCT AS 108-24-7  
SOL 67-56-1 MeOH, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 40 minutes, room temperature

PRO CB 503831-05-8

RX (25) RCT CB 503831-05-8  
PRO AU 503831-07-0  
CAT 14221-01-3 Pd(PPh<sub>3</sub>)<sub>4</sub>  
SOL 109-99-9 THF  
CON overnight, room temperature

RX (16) RCT BA 68858-20-8

STAGE (1)  
RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol  
SOL 872-50-4 NMEP  
CON 1 hour, room temperature

STAGE (2)  
RGT BJ 7087-68-5 EtN(Pr-i)<sub>2</sub>, BK 872-50-4 NMEP  
SOL 108-24-7 Ac<sub>2</sub>O

STAGE (3)  
RCT BB 71989-35-0  
RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol  
SOL 872-50-4 NMEP  
CON 1 hour, room temperature

STAGE (4)  
RGT BJ 7087-68-5 EtN(Pr-i)<sub>2</sub>, BK 872-50-4 NMEP  
SOL 108-24-7 Ac<sub>2</sub>O

STAGE (5)  
RCT BC 71989-33-8

RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol  
SOL 872-50-4 NMEP  
CON 1 hour, room temperature

STAGE (6)

RGT BJ 7087-68-5 EtN(Pr-i)2, BK 872-50-4 NMEP  
SOL 108-24-7 Ac2O

STAGE (7)

RCT BD 35661-39-3  
RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol  
SOL 872-50-4 NMEP  
CON 1 hour, room temperature

STAGE (8)

RGT BJ 7087-68-5 EtN(Pr-i)2, BK 872-50-4 NMEP  
SOL 108-24-7 Ac2O

STAGE (9)

STAGE (10)

RCT BE 132388-59-1  
RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol  
SOL 872-50-4 NMEP  
CON 1 hour, room temperature

STAGE (11)

RGT BJ 7087-68-5 EtN(Pr-i)2, BK 872-50-4 NMEP  
SOL 108-24-7 Ac2O

STAGE (12)

RGT BL 110-89-4 Piperidine  
SOL 872-50-4 NMEP  
CON 5 minutes, room temperature

STAGE (13)

RCT AU 503831-07-0  
RGT BM 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,  
1-[bis(dimethylamino)methylene]-, hexafluorophosphate(1-),  
3-oxide, BJ 7087-68-5 EtN(Pr-i)2  
SOL 872-50-4 NMEP

STAGE (14)

RCT BF 71989-31-6  
RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol  
SOL 872-50-4 NMEP  
CON 1 hour, room temperature

STAGE (15)

RGT BJ 7087-68-5 EtN(Pr-i)2, BK 872-50-4 NMEP  
SOL 108-24-7 Ac2O

STAGE (16)

RGT K 76-05-1 F3CCO2H  
SOL 75-18-3 Me2S, 108-39-4 3-Methylphenol, 540-63-6 HSCH2CH2SH  
CON room temperature -> -15 deg C

STAGE (17)

RGT AW 1493-13-6 F3CSO2H  
CON 1 hour, -15 deg C

STAGE(18)

RGT AM 110-86-1 Pyridine  
SOL 60-29-7 Et2O

PRO BG 503831-12-7

NTE solid-supported reaction, Sieber amide resin used, alternative cleavage step showed

ACCESSION NUMBER: 139:365206 CASREACT

TITLE: Solid-phase synthesis of core 2 O-linked glycopeptide and its enzymatic sialylation

AUTHOR(S): Takano, Yutaka; Kojima, Naoya; Nakahara, Yuko; Hojo, Hironobu; Nakahara, Yoshiaki

CORPORATE SOURCE: Institute of Glycotechnology, Department of Applied Biochemistry, Tokai University, Hiratsuka-shi, Kanagawa, 259-1292, Japan

SOURCE: Tetrahedron (2003), 59(42), 8415-8427

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

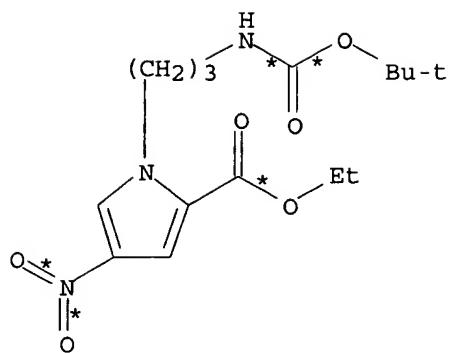
AB The core 2-type tetrasaccharide building blocks I (R = H, Me; R1 = Fmoc; R2 = OH) for solid-phase synthesis of glycopeptide were synthesized via stereoselective glycosylation of the disaccharyl Ser/Thr II (All = allyl) with a glycosyl fluoride III carrying the 2-trichloroacetamido group that was readily converted into a 2-acetamido group by reduction. Using building block I (R = Me, R1 = Fmoc, R2 = OH), a segment of glycoprotein leukosialin(215-224) I (R = Me, R1 = Fmoc-Pro-, R2 = -Thr-Ser-Thr-Asn-Ala-Ser-Thr-Val-NH2) was synthesized by the solid-phase protocol. Cleavage of the synthetic glycopeptide from resin was accomplished with reagent K and subsequent treatment of the product with a cocktail for the "low-acidity TfOH" facilitated complete removal of the benzyl groups with min. loss of glycosidic linkages. To the above glycopeptide, following Fmoc deprotection, N-acetylneurameric acid (sialic acid) residues were enzymically introduced in remarkably high efficiency by using the specific sialyltransferases.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

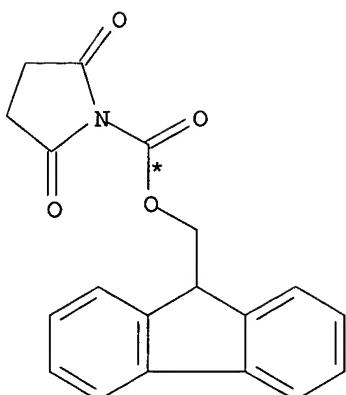
L11 ANSWER 5 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

RX(10) OF 10 COMPOSED OF RX(1), RX(2), RX(3), RX(4)

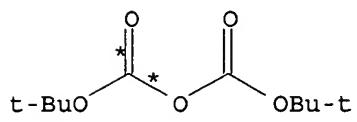
RX(10) A + B + P + R + S + T + U + V ==> W



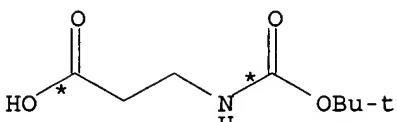
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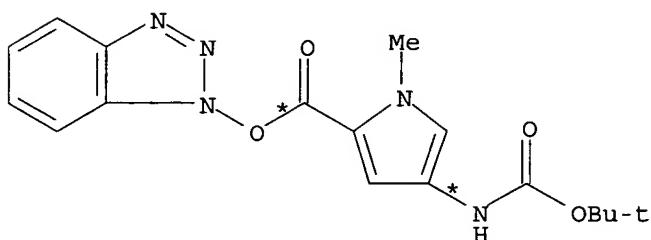
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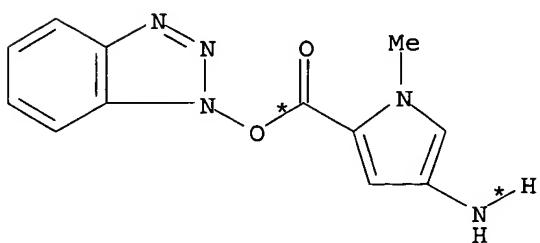
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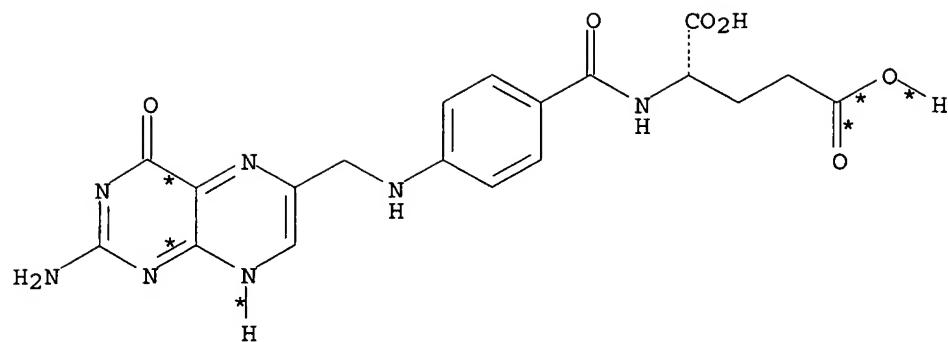
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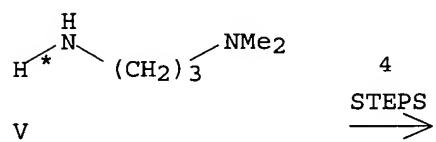
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T

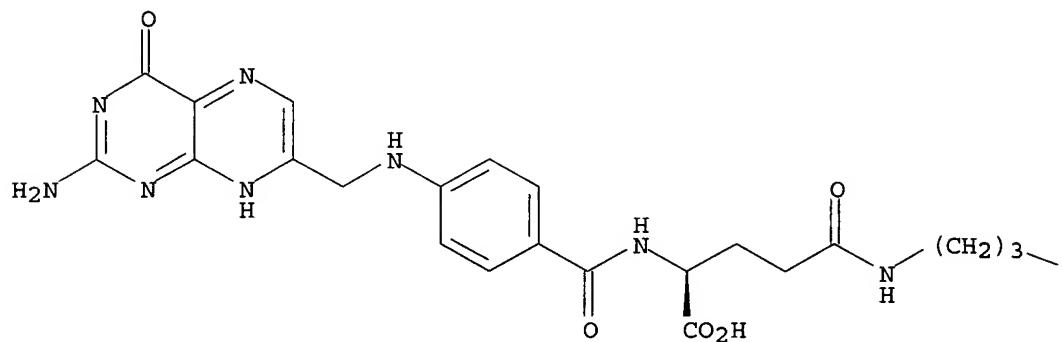


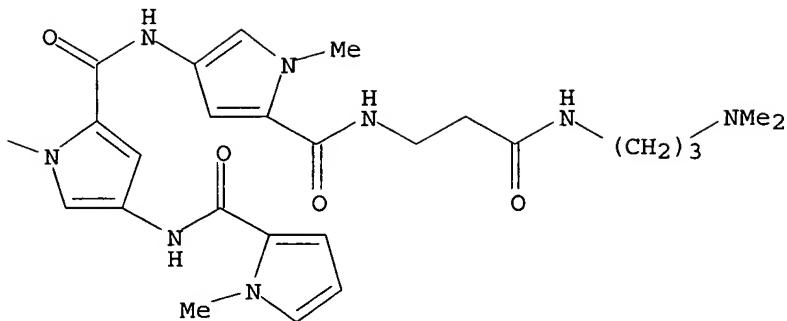
U



4  
STEPS  
→

PAGE 1-A





W  
YIELD 60%

RX (1) RCT A 159539-42-1

STAGE (1)

RGT D 1310-73-2 NaOH  
SOL 7732-18-5 Water, 64-17-5 EtOH

STAGE (2)

RGT E 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE (3)

RGT F 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2  
CON 2 hours, 0 deg C -> room temperature

STAGE (4)

RCT B 102774-86-7  
RGT G 497-19-8 Na2CO3  
SOL 67-64-1 Me2CO, 7732-18-5 Water  
CON 12 hours

PRO C 481070-51-3

RX (2) RCT C 481070-51-3  
RGT M 1333-74-0 H2  
PRO L 481070-49-9  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH  
CON 2 hours

RX (3) RCT L 481070-49-9, P 24424-99-5  
PRO Q 481070-50-2  
SOL 67-56-1 MeOH  
CON 2 hours, room temperature

RX (4) RCT R 3303-84-2D

STAGE(1)

RGT F 76-05-1 F3CCO2H, X 108-98-5 PhSH  
SOL 75-09-2 CH2Cl2

STAGE(2)

RCT S 77716-16-6  
RGT Y 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 90 minutes

STAGE(3)

RGT F 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2

STAGE(4)

RCT Q 481070-50-2  
RGT Z 2592-95-2 1-Benzotriazolol, AA 538-75-0 DCC, Y 7087-68-5  
EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 90 minutes

STAGE(5)

RGT F 76-05-1 F3CCO2H, X 108-98-5 PhSH  
SOL 75-09-2 CH2Cl2

STAGE(6)

RCT T 481070-52-4  
RGT Y 7087-68-5 EtN(Pr-i)2  
SOL 68-12-2 DMF  
CON 90 minutes

STAGE(7)

RCT U 59-30-3  
RGT AB 110-89-4 Piperidine, AC 872-50-4  
NMEP, AA 538-75-0 DCC, Z 2592-95-2 1-Benzotriazolol, Y  
7087-68-5 EtN(Pr-i)2  
CON 5 hours

STAGE(8)

RCT V 109-55-7  
CON 5 hours, 55 deg C

PRO W 481070-53-5  
NTE solid-state reaction, first stage attachment to  
Boc- $\beta$ -alanine-Pam resin

ACCESSION NUMBER: 138:73505 CASREACT  
TITLE: Solid-phase synthesis of a folate conjugate of a DNA  
binding polyamide  
AUTHOR(S): Sharma, Sanjay K.; Lown, J. William  
CORPORATE SOURCE: Department of Chemistry, University of Alberta,  
Edmonton, AB, T6G 2G2, Can.  
SOURCE: Tetrahedron Letters (2002), 43(37), 6665-6667  
CODEN: TELEAY; ISSN: 0040-4039  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

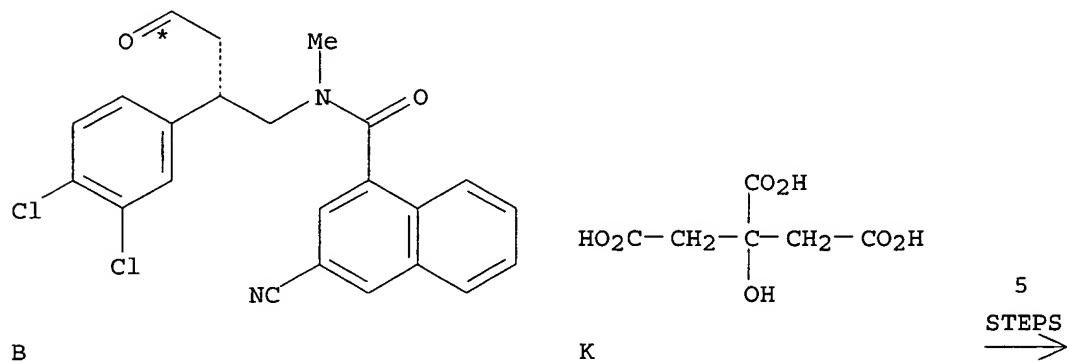
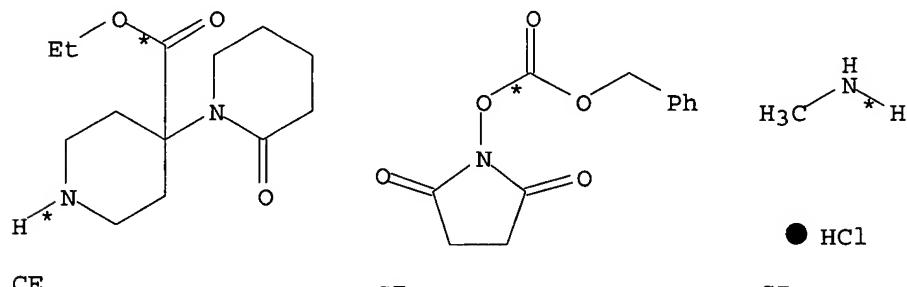
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

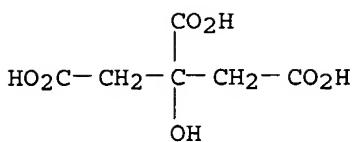
AB Solid-phase synthesis of a folate tripyrrolocarboxamide conjugate of a DNA binding polyamide (I) by connecting N-methyloligo(pyrrole)polyamide to folic acid using new monomer (II) is described. The synthesis of a new building block monomer Boc-Py-[(CH<sub>2</sub>)<sub>3</sub>-NHFmoc] (Boc = tert-butoxycarbonyl, Fmoc = 9-fluorenylmethoxycarbonyl, Py = pyrrolidine) acid II is also reported.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

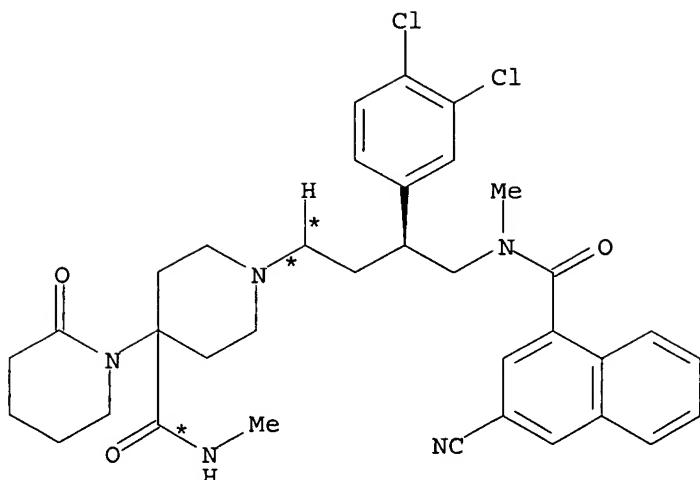
L11 ANSWER 6 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

RX(354) OF 425 COMPOSED OF RX(24), RX(25), RX(26), RX(17), RX(50)  
RX(354) CE + CF + CI + B + K ==> EI





EI: CM 1



EI: CM 2

RX (24) RCT CE 166180-90-1, CF 13139-17-8  
RGT BG 121-44-8 Et3N  
PRO CG 166180-93-4  
SQL 75-09-2 CH2Cl2

RX (25) RCT CG 166180-93-4  
RGT BA 1310-73-2 NaOH  
PRO CH 166180-94-5  
SQL 109-99-9 THE 7732-18-5 Water

RX(26) RCT CH 166180-94-5, CI 593-51-1  
RGT CJ 465535-95-9 1,3-Propanediamine, N'-carbonimidoyl-N,N-dimethyl-, monohydrochloride, CK 1122-58-3 4-DMAP  
PRO BP 166181-27-7  
SQL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(17) RCT BP 166181-27-7  
 RGT BQ 1333-74-0 H2  
 PRO O 166181-38-0  
 CAT 63310-18-9 Pd hydroxide  
 SOL 64-17-5 EtOH  
 NTE catalyst on carbon

RX(50) RCT B 255050-50-1, O 166181-38-0

STAGE (1)  
SOL 67-56-1 MeOH

STAGE (2)

STAGE (3)

STAGE (4)  
RGT R 144-55-8 NaHCO3  
SOL 7732-18-5 Water

STAGE (5)  
RCT K 77-92-9

PRO EI 255049-93-5

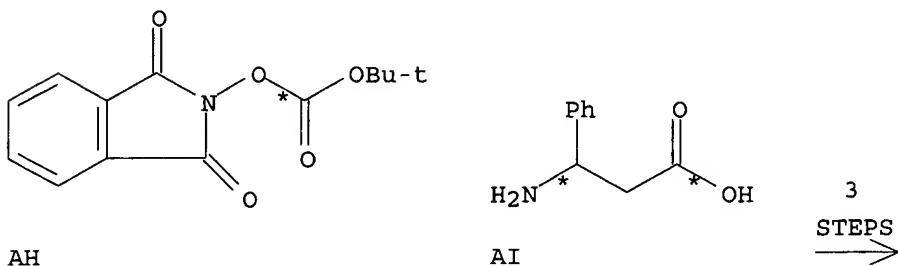
ACCESSION NUMBER: 137:272794 CASREACT  
TITLE: Design, Synthesis, and SAR of Tachykinin Antagonists: Modulation of Balance in NK1/NK2 Receptor Antagonist Activity  
AUTHOR(S): Albert, Jeffrey S.; Aharony, David; Andisik, Donald; Barthlow, Herbert; Bernstein, Peter R.; Bialecki, Russell A.; Dedinas, Robert; Dembofsky, Bruce T.; Hill, Daniel; Kirkland, Karin; Koether, Gerard M.; Kosmider, Benedict J.; Ohnmacht, Cyrus; Palmer, William; Potts, William; Rumsey, William; Shen, Lihong; Shenvi, Ashok; Sherwood, Scott; Warwick, Paul J.; Russell, Keith  
CORPORATE SOURCE: CNS Discovery Research, AstraZeneca Pharmaceuticals LP, Wilmington, DE, 19850-5437, USA  
SOURCE: Journal of Medicinal Chemistry (2002), 45(18), 3972-3983  
CODEN: JMCMAR; ISSN: 0022-2623  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

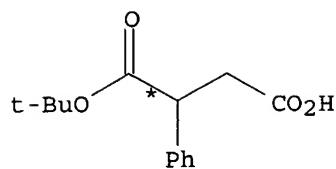
AB Through optimization of compds. based on the dual NK1/NK2 antagonist ZD6021, it was found that alteration of two key regions could modulate the balance of NK1 and NK2 potency. Substitution of the 2-naphthalene position in analogs of ZD6021 resulted in increased NK1 potency and thus afforded NK1 preferential antagonists. Alterations of the piperidine region could then increase NK2 potency to restore dual NK1/NK2 selectivity. Through these efforts, three novel receptor antagonists from a single chemical related series were identified; two are dual NK1/NK2 antagonists, and the third is an NK1 preferential antagonist. In this paper, the factors affecting the balance of NK1 and NK2 selectivity in this series are discussed and the in vitro and in vivo properties of the novel antagonists are described.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

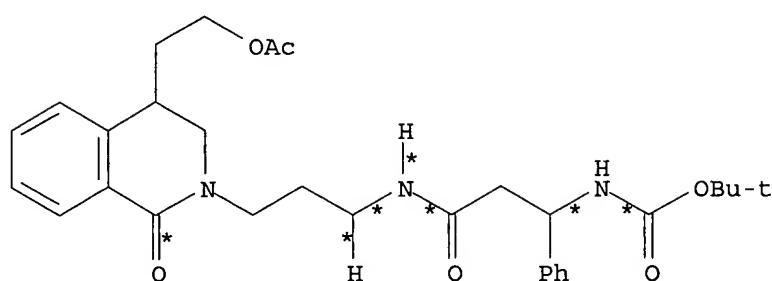
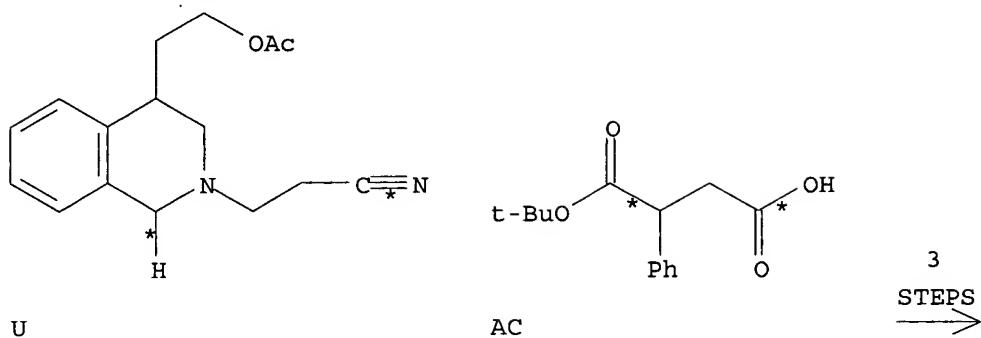
RX(42) OF 199 COMPOSED OF REACTION SEQUENCE RX(9), RX(8)  
AND REACTION SEQUENCE RX(6), RX(7), RX(8)  
...AH + AI ==> AC...  
... U + AC ==> AD





AC

START NEXT REACTION SEQUENCE



AD

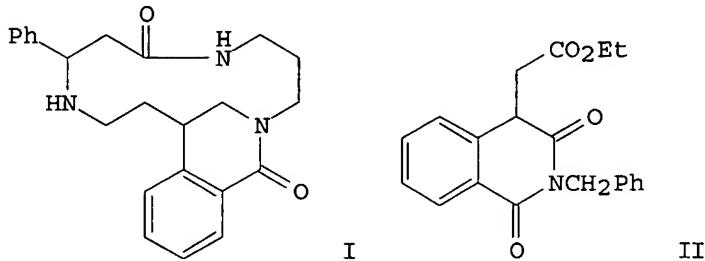
RX (9) RCT AH 15263-20-4, AI 614-19-7  
PRO AC 104465-81-8  
SOL 68-12-2 DMF, 7732-18-5 Water

RX(6) RCT U 104465-78-3  
RGT W 7722-64-7 KMnO<sub>4</sub>, X 7487-88-9 MgSO<sub>4</sub>  
PRO V 104465-79-4  
SOL 67-64-1 Me<sub>2</sub>CO, 7732-18-5 Water

RX(7)	RCT	V 104465-79-4
	RGT	L 1333-74-0 H2
	PRO	Z 104465-80-7
	CAT	11129-89-8 Pt oxide
	SOL	67-66-3 CHCl3, 64-17-5 EtOH

RX(8) RCT AC 104465-81-8, Z 104465-80-7  
RGT AE 14338-32-0 2-Cl-py.MeI, AF 121-44-8 Et3N

PRO AD 104465-82-9  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
ACCESSION NUMBER: 106:5298 CASREACT  
TITLE: Total synthesis of  $\pm$ -isocycloelabenzene  
AUTHOR (S): Iida, Hideo; Fukuhara, Kiyoshi; Murayama, Yoshiaki;  
Machiba, Mitsuo; Kikuchi, Toyohiko  
CORPORATE SOURCE: Tokyo Coll. Pharm., Horinouchi Hachioji, 192-03, Japan  
SOURCE: Journal of Organic Chemistry (1986), 51(24), 4701-3  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The macrocyclic spermidine alkaloid isocyclocelabenzene (I) was synthesized from homophthalimide derivative II and 3-amino-3-phenylpropionic acid.

=> fil caplus;s werpy t?/au

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L12 28 WERPY T?/AU

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L13 263 FRYE J?/AU

L14 8093 WHITE J?/AU

L15 20 ZACHER A?/AU

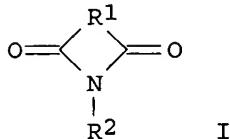
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L16 1 L12 AND L13 AND L14 AND L15

=> d ibib abs

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2004:566590 CAPLUS  
DOCUMENT NUMBER: 141:123556.  
TITLE: Process for producing N-methylsuccinimide from  
dicarbonyl compounds by cyclization and alkylation and  
hydrogenation to N-methylpyrrolidinone  
INVENTOR(S): Werpy, Todd A.; Frye, John G., Jr.  
; White, James F.; Holladay, Johnathan E.;  
Zacher, Alan H.  
PATENT ASSIGNEE(S): Battelle Memorial Institute, USA  
SOURCE: PCT Int. Appl., 31 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004058708	A1	20040715	WO 2003-US40106	20031216
WO 2004058708	B1	20040923		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004176589	A1	20040909	US 2003-731108	20031210
EP 1572644	A1	20050914	EP 2003-814062	20031216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRIORITY APPLN. INFO.:			US 2002-435469P	P 20021220

OTHER SOURCE(S) :	CASREACT 141:123556; MARPAT 141:123556	US 2003-108336	A 20031210
GI		US 2003-731108	A 20031210
		WO 2003-US40106	W 20031216



AB The invention includes methods of processing an initial di-carbonyl compound by conversion to a cyclic compound I (R<sup>1</sup> = linear or branched, saturated or unsatd. hydrocarbon or substituted hydrocarbon; R<sup>2</sup> = H; linear, cyclic or branched, saturated or unsatd. alkyl; aromatic group). The cyclic compound is reacted with an alkylating agent to form a derivative having an alkylated ring nitrogen. The invention encompasses a method of producing an N-alkyl product. Ammonia content of a solution is adjusted to produce a ratio of ammonia to dicarboxylate compound of from about 1:1 to about 1.5:1. An alkylating agent is added and the initial compound is alkylated and cyclized. The invention includes methods of making N-methylpyrrolidinone (NMP). Aqueous ammonia and succinate is introduced into a vessel and ammonia is adjusted to provide a ratio of ammonia to succinate of less than 2:1. A methylating agent is reacted with succinate at a temperature of from greater than 100° to about 400° to produce N-methylsuccinimide which is purified and hydrogenated to form NMP.

=> s (l12 or l13 or l14 or l15) and ?succinimide?

30895 ?SUCCINIMIDE?

L17 7 (L12 OR L13 OR L14 OR L15) AND ?SUCCINIMIDE?

=> d 1-7 ibib abs hitstr

L17 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:566590 CAPLUS

DOCUMENT NUMBER: 141:123556

TITLE: Process for producing N-methylsuccinimide from dicarbonyl compounds by cyclization and alkylation and hydrogenation to N-methylpyrrolidinone

INVENTOR(S): Werpy, Todd A.; Frye, John G., Jr.  
; White, James F.; Holladay, Johnathan E.;  
Zacher, Alan H.

PATENT ASSIGNEE(S): Battelle Memorial Institute, USA

SOURCE: PCT Int. Appl., 31 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

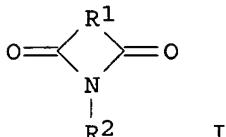
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004058708	A1	20040715	WO 2003-US40106	20031216

WO 2004058708	B1	20040923		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004176589	A1	20040909	US 2003-731108	20031210
EP 1572644	A1	20050914	EP 2003-814062	20031216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRIORITY APPLN. INFO.:			US 2002-435469P	P 20021220
			US 2003-108336	A 20031210
			US 2003-731108	A 20031210
			WO 2003-US40106	W 20031216
OTHER SOURCE(S):	CASREACT 141:123556; MARPAT 141:123556			
GI				



AB The invention includes methods of processing an initial di-carbonyl compound by conversion to a cyclic compound I (R<sup>1</sup> = linear or branched, saturated or unsatd. hydrocarbon or substituted hydrocarbon; R<sup>2</sup> = H; linear, cyclic or branched, saturated or unsatd. alkyl; aromatic group). The cyclic compound is reacted with an alkylating agent to form a derivative having an alkylated ring nitrogen. The invention encompasses a method of producing an N-alkyl product. Ammonia content of a solution is adjusted to produce a ratio of ammonia to dicarboxylate compound of from about 1:1 to about 1.5:1. An alkylating agent is added and the initial compound is alkylated and cyclized. The invention includes methods of making N-methylpyrrolidinone (NMP). Aqueous ammonia and succinate is introduced into a vessel and ammonia is adjusted to provide a ratio of ammonia to succinate of less than 2:1. A methylating agent is reacted with succinate at a temperature of from greater than 100° to about 400° to produce N-methylsuccinimide which is purified and hydrogenated to form NMP.

L17 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2002:977786 CAPLUS  
 DOCUMENT NUMBER: 138:57825  
 TITLE: Method and catalysts of making pyrrolidones by hydrogenation  
 INVENTOR(S): Werpy, Todd; Frye, John G., Jr.;  
 Wang, Yong; Zacher, Alan H.  
 PATENT ASSIGNEE(S): Battelle Memorial Institute, USA  
 SOURCE: PCT Int. Appl., 44 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002102772	A1	20021227	WO 2002-US19372	20020617
WO 2002102772	B1	20031120		
W: AE, AG, AL, AM, AT, AU, AZ, CR, CU, CZ, DE, DK, DM, DZ, HU, ID, IL, IN, IS, JP, KE, LU, LV, MA, MD, MG, MK, MN, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, ZA, ZW	BA, BB, BG, BR, BY, BZ, CA, CH, CN, EE, ES, FI, GB, GD, GE, GH, GM, HR, KG, KP, KR, KZ, LC, LK, LR, LS, LT, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SE, TR, TZ, UA, UG, UZ, VN, YU,			
RW: GH, GM, KE, LS, MW, MZ, SD, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2003097006	A1	20030522	US 2001-884602	20010618
US 6603021	B2	20030805		
EP 1412329	A1	20040428	EP 2002-756233	20020617
R: AT, BE, CH, DE, DK, ES, FR, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR	GB, GR, IT, LI, LU, NL, SE, MC, PT,			
US 2003114687	A1	20030619	US 2002-280577	20021025
US 6706893	B2	20040316		
US 2003120087	A1	20030626	US 2002-280462	20021025
US 6670483	B2	20031230		
US 2003125570	A1	20030703	US 2002-280622	20021025
US 6632951	B2	20031014		
PRIORITY APPLN. INFO.:			US 2001-884602	A 20010618
			WO 2002-US19372	W 20020617

OTHER SOURCE(S): MARPAT 138:57825

AB The present invention provides methods for making N-methylpyrrolidine and analogous compds. via hydrogenation. Catalysts for this process comprise carbon, metal oxides, and Pd, Rh, Pt, Ru, Ni, and/or Co. Other process improvements may include extraction and hydrolysis steps. Some preferred reactions take place in the aqueous phase. Starting materials for making N-methylpyrrolidine may include succinic acid, N-methylsuccinimide, and their analogs.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:962011 CAPLUS

DOCUMENT NUMBER: 138:154086

TITLE: Neutron and X-ray Reflectivity from Polyisobutylene-Based Amphiphiles at the Air-Water Interface

AUTHOR(S): Reynolds, Philip A.; McGillivray, Duncan J.; Gilbert, Elliot P.; Holt, Stephen A.; Henderson, Mark J.; White, John W.

CORPORATE SOURCE: Research School of Chemistry, The Australian National University, Canberra, 0200, Australia

SOURCE: Langmuir (2003), 19(3), 752-761

CODEN: LANGD5; ISSN: 0743-7463

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have performed X-ray and neutron reflectivity expts. on amphiphile films spread at the air-water and air-saturated ammonium nitrate solution

interfaces as a function of film compression. We have examined ca. 750, 1100, and 1700 mol. weight monodisperse polyisobutylene amide (PIBSA), 1100 imide (PIBSIM), and also palmitic acid for the pure amphiphiles and binary mixts. We have used deuterated and hydrogenous components so that a given film may be examined in up to seven contrasts. All of the films form a monolayer, with mol. area determined by tail group size, which increases slightly in thickness on compression for PIB derivs. There are differences in film thicknesses as shown by a dependence on compression and substructure; this is understood in terms of the increasing tendency of the tail to adopt a coiled conformation as mol. weight increases. PIBSA films consist of packed micrometer scale disks containing up to 10% open water (polynya) area. Palmitic acid-containing films contain a greater polynya area. All films lose up to half of the original amount of amphiphile from the monolayer when compressed. The almost reversible loss of material followed the trend palmitic acid < 750 amide < 1100 amide < 1100 imide, empirically in order of hydrophile-lipophile balance (HLB) number. This pattern suggests an amphiphile loss into submicrometer aggregates at the interface, rather than dispersion into the aqueous phase. Binary mixts. exhibit differential competition of the components to remain in the monolayer with the trend: palmitic acid > 750 amide > 1100 amide > 1100 imide, opposite to the aggregation tendency as expected. The preference to remain at the surface may be phys. related to more effective packing of the headgroup mols. on the surface when head and tail areas are better matched in size. Mixts. also spontaneously segregate laterally and form micrometer scale domains. This tendency also follows the HLB number, with better mixing for those components with similar HLB values. Lateral segregation is encouraged by film compression. Surprisingly, properties of films on water and 50 wt% ammonium nitrate subphase show little difference with respect to these trends.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2001:541397 CAPLUS  
 DOCUMENT NUMBER: 135:344623  
 TITLE: Asymmetric synthesis of (+)-loline, a pyrrolizidine alkaloid from rye grass and tall fescue  
 AUTHOR(S): Blakemore, Paul R.; Kim, Sung-Kee; Schulze, Volker K.; White, James D.; Yokochi, Alexandre F. T.  
 CORPORATE SOURCE: Department of Chemistry, Oregon State University, Corvallis, OR, 97331-4003, USA  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2001), (15), 1831-1847  
 CODEN: JCSPCE; ISSN: 1472-7781  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:344623  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB (+)-Loline (I) was synthesized via a pathway that employed intramol. [4 + 2] cycloaddn. of an acylnitrosodiene, (S,E)-H<sub>2</sub>C:CHCH:CHCH(OR<sub>1</sub>)CH<sub>2</sub>CON:O (R<sub>1</sub> = SiMe<sub>2</sub>CMe<sub>3</sub>, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>OMe-4), as a key step. The acylnitrosodienes, which were used in situ, were obtained by oxidation of the corresponding hydroxamic acids, (S,E)-H<sub>2</sub>C:CHCH:CHCH(OR<sub>2</sub>)CH<sub>2</sub>CONHOH (R<sub>2</sub> = SiMe<sub>2</sub>CMe<sub>3</sub>, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>OMe-4),

and these were prepared from either glucose via aldehyde II or more directly from (S)-malic acid. The endo dihydrooxazines III (R3 = SiMe<sub>2</sub>CMe<sub>3</sub>, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>OMe-4), obtained in a mixture with their exo stereoisomer, were transformed by reductive N-O bond cleavage and reannulation into pyrrolizines IV (R4 = SiMe<sub>2</sub>CMe<sub>3</sub>, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>OMe-4). The latter was subjected to Sharpless aminohydroxylation in the presence of (DHQD)<sub>2</sub>PHAL to give V (R5 = R6 = H) along with its regioisomer. N-Methylation of tosyl amide V (R5 = R6 = H), followed by mesylation of alc. V (R5 = H; R6 = Me) and reduction of the  $\gamma$ -lactam V (R5 = SO<sub>2</sub>Me; R6 = Me) with borane, afforded pyrrolizidine VI (R7 = CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>OMe-4). Cleavage of the p-methoxybenzyl ether and subsequent thermal treatment of VI (R7 = H) resulted in intramol. etherification to yield N-tosylloline (VII). Final reductive cleavage of the N-tosyl residue produced (+)-loline (I), characterized as its dihydrochloride.

REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:441402 CAPLUS

DOCUMENT NUMBER: 107:41402

TITLE: Synthesis of a new thermally curable elastomer via regioselective chlorination of a polyimidosulfide

AUTHOR(S): White, Jerry E.

CORPORATE SOURCE: Cent. Res.-Polym. Mater. Lab., Dow Chem. Co., Midland, MI, 48674, USA

SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry (1987), 25(4), 1191-5

CODEN: JPACCEC; ISSN: 0887-624X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The title rubber was synthesized from the reaction of N-chlorosuccinimide with a polyimidosulfide which was prepared by polymerization of 1,4-butanediol and N,N'-bismaleimido-1,8-octane. NMR spectrum

showed a vinyl proton absorption at  $\delta$  = 5.90 whose integration along with integrations of ring CH and CH<sub>2</sub> protons were consistent with the composition

L17 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:406776 CAPLUS

DOCUMENT NUMBER: 103:6776

TITLE: Step-growth polymers from bismaleimides. Synthesis and reactions of some new polyimides

AUTHOR(S): White, Jerry E.; Scaia, Mark D.; Snider-Tung, Deborah A.

CORPORATE SOURCE: Cent. Res., Dow Chem. Co., Midland, MI, 48640, USA

SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1985), 26(1), 132-3

CODEN: ACPPAY; ISSN: 0032-3934

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Linear high-mol.-weight polyaspartimide were prepared in 58-84% yield by poly addition of N,N'-dimethyl-1,6-hexanediamine or piperazine with bismaleimides. Polyimidosulfides in 75-86% yield were prepared by addition of dithiols with bismaleimides.

L17 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:48570 CAPLUS

DOCUMENT NUMBER: 102:48570

TITLE: Soluble oil cutting fluid

INVENTOR(S) : Rawlinson, Anthony Paul; White, James  
PATENT ASSIGNEE(S) : British Petroleum Co. PLC, UK  
SOURCE: Eur. Pat. Appl., 11 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 120665	A2	19841003	EP 1984-301863	19840320
EP 120665	A3	19850403		
EP 120665	B1	19870513		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
AU 8425867	A1	19840927	AU 1984-25867	19840319
AU 558608	B2	19870205		
AT 27174	E	19870515	AT 1984-301863	19840320
CA 1223243	A1	19870623	CA 1984-450069	19840321
DK 8401632	A	19840924	DK 1984-1632	19840322
ZA 8402146	A	19851127	ZA 1984-2146	19840322
PRIORITY APPLN. INFO.:			GB 1983-7975	A 19830323
			EP 1984-301863	A 19840320

AB A soluble-oil concentrate, to be diluted with H<sub>2</sub>O, comprises an alkali or alkaline-earth alkylbenzenesulfonate, a fatty acid diethanolamide, a mixed alkanolamine borate, a polyisobutene derivative of succinimide, and mineral oil. The soluble oil is stable without containing a conventional coupling agent, some soluble-oil emulsions are biostatic, even though conventional biocides are not included.

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(FILE 'HOME' ENTERED AT 16:10:59 ON 31 JAN 2006)

FILE 'CASREACT' ENTERED AT 16:11:08 ON 31 JAN 2006

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L2 STR L1  
L3 0 S L2  
L4 2 S L2 FUL  
L5 6 S WERPY ?/AU

FILE 'CASREACT' ENTERED AT 16:20:25 ON 31 JAN 2006

L6 STR L3  
L7 50 S L6  
L8 2816 S L6 FUL  
L9 STR L2  
L10 9 SEARCH L9 SUB=L8 FUL  
L11 7 S L10 NOT L4

FILE 'CAPLUS' ENTERED AT 16:23:27 ON 31 JAN 2006

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L13 263 S FRYE J?/AU  
L14 8093 S WHITE J?/AU  
L15 20 S ZACHER A?/AU  
L16 1 S L12 AND L13 AND L14 AND L15  
L17 7 S (L12 OR L13 OR L14 OR L15) AND ?SUCCINIMIDE?

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FULL ESTIMATED COST	33.97	337.07
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.00	-16.65

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DICTIONARY FILE UPDATES: 30 JAN 2006 HIGHEST RN 873057-98-8

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\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
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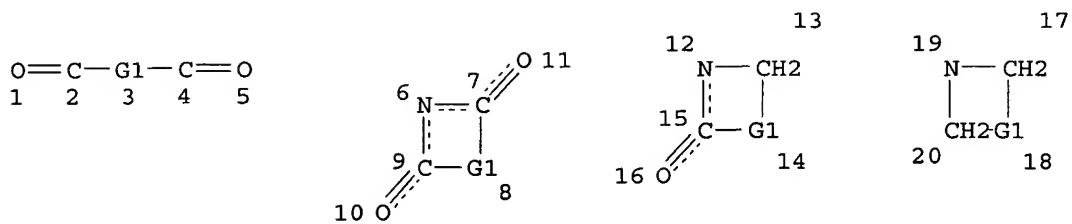
Structure search iteration limits have been increased. See HELP SLIMITS  
for details.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

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E2 1 N-METHYL PROSCILLARIDIN A LACTAM/CN  
E3 0 --> N-METHYL SUCCINIMIDE/CN  
E4 1 N-METHYL TAXOL A/CN  
E5 1 N-METHYL TETRAFLUOROPHTHALIMIDE/CN

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L2 STR



REP G1=(2-4) C

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

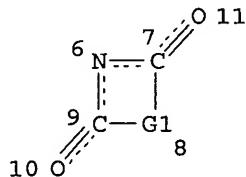
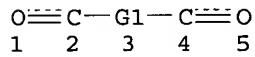
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100.0% DONE    73794 VERIFIED    42 HIT RXNS

2 DOCS

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L6                    STR



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NODE ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

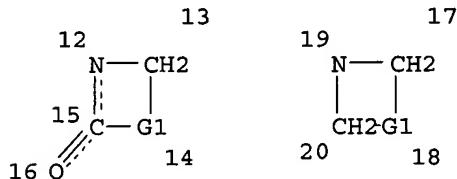
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NUMBER OF NODES IS 11

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L9                    STR



REP G1=(2-4) C

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
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NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE  
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100.0% DONE 51070 VERIFIED 124 HIT RXNS 9 DOCS  
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(FILE 'HOME' ENTERED AT 16:10:59 ON 31 JAN 2006)

FILE 'CASREACT' ENTERED AT 16:11:08 ON 31 JAN 2006

L1 STR  
L2 STR L1  
L3 0 S L2  
L4 2 S L2 FUL  
L5 6 S WERPY ?/AU

FILE 'CASREACT' ENTERED AT 16:20:25 ON 31 JAN 2006

L6 STR L3  
L7 50 S L6  
L8 2816 S L6 FUL  
L9 STR L2  
L10 9 SEARCH L9 SUB=L8 FUL  
L11 7 S L10 NOT L4

FILE 'CAPLUS' ENTERED AT 16:23:27 ON 31 JAN 2006

L12 28 S WERPY T?/AU  
L13 263 S FRYE J?/AU  
L14 8093 S WHITE J?/AU  
L15 20 S ZACHER A?/AU  
L16 1 S L12 AND L13 AND L14 AND L15  
L17 7 S (L12 OR L13 OR L14 OR L15) AND ?SUCCINIMIDE?

FILE 'REGISTRY' ENTERED AT 16:26:43 ON 31 JAN 2006  
E "N-METHYL SUCCINIMIDE"/CN 5

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.44	337.51
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-16.65

STN INTERNATIONAL LOGOFF AT 16:27:24 ON 31 JAN 2006